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CLUJ, OMEGA AND RELATED POLYNOMIALS IN TORI T(4,4)R[*c*,*n*]

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ABSTRACT. Cluj and Omega polynomials were designed to describe the graphs associated to polyhedral nanostructures: their exponents express the extent of partitions of a graph property while the coefficients count the partitions of a given extent. Basic definitions and properties of these and some other related counting polynomials are given, as derived from the cutting procedure of their calculation. Formulas to calculate these polynomials in T(4,4)R[*c*,*n*] tori are given and exemplified.

Keywords: *Cluj polynomial, Omega polynomial, nanotori*

POLYNOMIALS IN CHEMISTRY

One of the most used representations of a molecular graph is that of a polynomial. In Quantum Chemistry, the early Hückel theory made use of the *characteristic polynomial* in calculating the levels of π-electron energy of the molecular orbitals, in conjugated hydrocarbons [1-4]:

$$Ch(x) = \det[x\mathbf{I} - \mathbf{A}] \tag{1}$$

In the above, **I** is the unit matrix of a pertinent order and **A** the adjacency matrix of the graph *G*. The characteristic polynomial is involved in the evaluation of topological resonance energy TRE, the topological effect on molecular orbitals TEMO, the aromatic sextet theory, the Kekulé structure count, *etc*. [4-8]

A general form of a counting polynomial is the following:

$$P(\mathbf{M}, x) = \sum_k m(k) \cdot x^k \tag{2}$$

where the exponents represent the extent of partitions *p*(*G*), $\cup\, p(G) = P(G)$ of a graph property *P*(*G*) while the coefficients $m(k)$ are related to the number of

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partitions of extent *k*. In relation (2), the coefficients $m(k)$ are calculable from the graph *G* by a method making use of the *Sachs graphs*, which are subgraphs of *G*. Some numeric methods of linear algebra, can eventually be more efficient in large graphs [9,10]. More about the characteristic polynomial, the reader can find in ref [1].

In the Mathematical Chemistry literature, the counting polynomials have been introduced by Hosoya [11,12] and later by other scientists [12,21].

POLYNOMIALS OF VERTEX PROXIMITY

Cluj polynomials are defined [22-25] on the basis of vertex proximities p_i,

$$P(\mathbf{UCJ}, x) = \sum_k m(k) \cdot x^k \qquad (3)$$

where summation runs over all $k = |\{p\}|$ in *G* with *p* being the proximity of the vertex *i* with respect to any vertex *j* in *G*, joined to *i* by an edge $\{p_{e,i}\}$ (the Cluj-edge polynomials) or by a path $\{p_{p,i}\}$ (the Cluj-path polynomials), taken as the shortest (*i.e.*, distance DI) or the longest (*i.e.*, detour DE) paths.

In (3), the coefficients *m*(*k*) can be calculated from the entries in the non-symmetric Cluj matrices (as provided by the TOPOCLUJ software program) [26] which represent vertex proximities. To define these, we need some theoretical background, as follows.

A graph *G* is a *partial cube* if it is embeddable in the *n*-cube Q_n, which is the regular graph whose vertices are all binary strings of length *n*, two strings being adjacent if they differ in exactly one position [27]. The distance function in the *n*-cube is the Hamming distance. A hypercube can also be expressed as the Cartesian product: $Q_n = \square_{i=1}^{n} K_2$. A subgraph $H \subseteq G$ is called *isometric*, if $d_H(u,v) = d_G(u,v)$, for any $(u,v) \in H$; it is *convex* if any shortest path in *G* between vertices of *H* belongs to *H*.

For any edge *e*=(*u*,*v*) of a connected graph *G* let n_{uv} denote the set of vertices lying closer to *u* than to *v*: $n_{uv} = \{ w \in V(G) \mid d(w,u) < d(w,v) \}$. It follows that $n_{uv} = \{ w \in V(G) \mid d(w,v) = d(w,u) + 1 \}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu}, are called *semicubes* of *G*; the semicubes are called *opposite semicubes* and are disjoint [28].

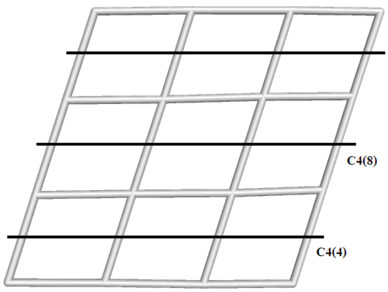
A graph *G* is bipartite if and only if, for any edge of *G*, the opposite semicubes define a partition of *G*: $n_{uv} + n_{vu} = v = |V(G)|$. These semicubes are just the vertex proximities of (the endpoints of) edge *e*=(*u*,*v*), which *CJ* polynomial counts. In partial cubes, the semicubes can be estimated by an orthogonal edge-cutting procedure.

The orthogonal cuts form a partition of the edges in *G*:

$$E(G) = c_1 \cup c_2 \cup ... \cup c_k,\ \ c_i \cap c_j = \varnothing, i \neq j\ .$$

To perform an orthogonal edge-cutting [25,29-32] take a straight line segment, orthogonal to the edge *e*, and intersect *e* and all its parallel edges (in a polygonal plane graph). The set of these intersections is called an *orthogonal cut* c_k, k=1,2,..,k_{max} of *G*, with respect to the edge *e* (Figure 1). To any orthogonal cut c_k, two numbers are associated: first one represents the *number of edges* e_k "cut-off", or the cutting cardinality $|\ c_k\ |$ while the second (in round brackets, in Figure 1) is v_k or the number of points lying to the left hand with respect to c_k.

Cluj and some related polynomials are calculable from the semicubes in *G* (see the polynomial exponents, Figure 1), they differing only in the mathematical operation used in composing the edge contributions to the global graph property. Because, in a bipartite graph, the opposite semicubes define a partition of vertices, it is easily to identify the two semicubes: $n_{uv} = v_k$ and $n_{vu} = v - v_k$ or vice-versa.



$CJ\ S(x) = 2·2·4(x^4+x^{12}) + 2·1·4(x^8+x^8)$
$= 16x^4+16x^8+16x^{12}$
$CJ\ S'(1) = 384;$
$PI_v(x) = 2·2·4(x^{4+12}) + 2·1·4(x^{8+8})$
$=16x^{16} + 8x^{16} = 24x^{16};$
$PI_v'(1) = 384;$

$CJ\ P(x) = 2·2·4(x^{4·12}) + ·1·4(x^{8·8})$
$= 16x^{48} + 8x^{64} = SZ(x)$
$CJ\ P'(1) = 1280 = SZ'(1);$

$\Omega(x) = (2·3)x^4$
$\Omega'(1) = 24 = e = |E(G)|$
$CI(G) = 480;$
$\Theta(x) = 4(2·3)x^4$
$\Theta'(1) = 96;$
$\Pi(x) = 4(2·3)x^{20}$
$\Pi'(1) = 480 = PI'(1)$

Figure 1. Calculating of several topological descriptors by the Cutting procedure

The coefficients of these descriptors are calculated (with some exceptions) as the product of three numbers (in the front of brackets - right hand part of Figure 1) with the meaning: (i) symmetry of *G*; (ii) occurrence of c_k (in the whole structure) and (iii) e_k.

According to the mathematical operation used in composing the graph semicubes, four polynomials can be defined:

(i) *Summation*, and the polynomial is called *Cluj-Sum*, by Diudea *et al*. [22-25,31-33] (and symbolized CJ_eS):

$$CJ_eS(x) = \sum_e \left(x^{v_k} + x^{v-v_k} \right) \tag{4}$$

(ii) *Pair-wise summation*, with the polynomial called (vertex) Padmakar-Ivan [34] by Ashrafi [35-38] (and symbolized PI_v):

$$PI_v(x) = \sum_e x^{v_k + (v - v_k)} \tag{5}$$

(iii) *Pair-wise product*, while the polynomial is called *Cluj-Product* (and symbolized CJ_eP) [25,31,39-43] or also *Szeged* polynomial (and symbolyzed *SZ*) [36-38]:

$$CJ_eP(x) = SZ(x) = \sum_e x^{v_k (v - v_k)} \tag{6}$$

The first derivative (in x=1) of a (graph) counting polynomial provides single numbers, often called topological indices.

It is not difficult to see that the first derivative (in x=1) of the first two polynomials gives one and the same value; however, their second derivative is different and the following relations hold in any graph [24]:

$$CJ_eS'(1) = PI_v'(1)\,;\; CJ_eS''(1) \neq PI_v''(1) \tag{7}$$

The number of terms is given by the value of the polynomial in x=1: it is $CJ_eS(1)=2e$ and $PI_v(1)=e$, respectively, because in the last case the two endpoint contributions are pair-wise summed for any edge in a bipartite graph.

Observe the first derivative (in x=1) of $PI_v(x)$ takes the maximal value in bipartite graphs:

$$PI_v'(1) = e \cdot v = |E(G)| \cdot |V(G)| \tag{8}$$

It can also be seen by considering the definition of the corresponding index [44]:

$$PI_v(G) = PI_v'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V| \cdot |E| - \sum_{e=uv} m_{u,v} \tag{9}$$

where $n_{u,v}$, $n_{v,u}$ count the non-equidistant vertices with respect to the endpoints of the edge $e=(u,v)$ while $m(u,v)$ is the number of equidistant vertices *vs*. u and v. However, it is known that, in bipartite graphs, there are no equidistant vertices *vs*. any edge, so that the last term in (9) is null. The value of $PI_v(G)$ is thus maximal in bipartite graphs, among all graphs on the same number of vertices; the result of (8) can be used as a criterion for checking the "bipatity" of a graph.

The third polynomial uses the pair-wise product; notice that Cluj-Product $CJ_eP(x)$ is precisely the (vertex) Szeged polynomial $SZ_v(x)$, defined by Ashrafi *et al*. [36-38].This comes out from the relations between the basic Cluj (Diudea [39-41,45,46]) and Szeged (Gutman [46,47]) indices:

$$CJ_e P'(1) = CJ_e DI(G) = SZ(G) = SZ_v'(1) \tag{10}$$

These polynomials (and their derived indices) do not count the equidistant vertices, an idea introduced in Chemical Graph Theory by Gutman [47]. When subscript letter is missing, $SZ(x)$ is $SZ_v(x)$.

POLYNOMIALS OF VERTEX PROXIMITY IN RHOMB-TILED TORI

The covering (4,4)S, embedded in the torus, can be changed to the rhombic (4,4)R pattern by the Medial *Med* operation on maps [48].

$$Med(\mathrm{T}(4{,}4)\mathrm{S}[c,n]) \longrightarrow (\mathrm{T}(4{,}4)\mathrm{R}[2c,n]) \tag{11}$$

Since the *Med* operation will double the number of points in the original object (*i.e.*, the vertex multiplicity m =2), it is clear that these graphs are bipartite.

The cutting procedure can be applied in case of rhomb-tiled tori T(4,4)R[*c*,*n*]; each cutting provides halves, as illustrated in Figure 2. Table 1 includes both formulas and pertinent examples in this series.

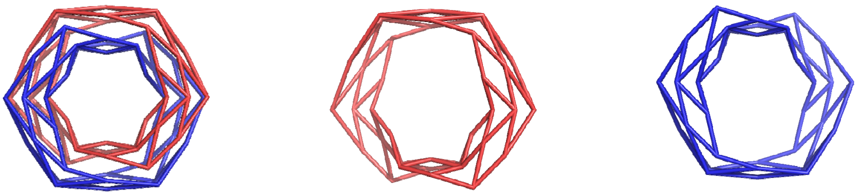


Figure 2. Cutting procedure in rhomb-tiled tori T(4,4)R[*c*,*n*]; the two halves are red/blue colored.

The rhomb-tiled tori are not partial cubes, then the cutting procedure cannot be applied in calculating the Wiener index $W(G)$ [30].

POLYNOMIALS OF EDGE PROXIMITY

Let $G=(V(G),E(G))$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = (u,v)$ and $f = (x,y)$ of G are called *co-distant* (briefly: e *co* f) if the notation can be selected such that [28,49]:

$$e\ co\ f \Leftrightarrow d(v,x) = d(v,y)+1 = d(u,x)+1 = d(u,y) \tag{12}$$

where d is the usual shortest-path distance function. Relation *co* is reflexive, that is, e *co* e holds for any edge e of G and it is also symmetric: if e *co* f then also f *co* e. In general, *co* is not transitive. A graph is called a *co-graph* if the relation *co* is transitive and thus an equivalence relation.

Table 1. Polynomials of vertex proximity in tori T(4,4)R[*c*,*n*] designed by Med(T(4,4)S[*c*,*n*]); vertex multiplicity *m*=2.

Formulas	
$CJS(x) = e(x^{v/2} + x^{v/2})$	$CJP(x) = SZ(x) = e(x^{v/2 \cdot v/2})$
$CJS'(1) = e(v/2 + v/2) = e \cdot v = 2(cn)^2$	$CJP'(1) = e(v/2 \cdot v/2) = e(v/2)^2$
$PI_v(x) = e(x^{v/2+v/2}) = e \cdot x^v$	$= (1/2)v^3 = (1/2)(cn)^3$
$PI_v'(1) = e \cdot v = CJ_eS'(1)$	$v = cn$; $e = 2c \cdot 2n$

Examples
Med(T(4,4)S[5,10]): CJS(x)=400x^50; P`(1)=20000; $PI_v$(x)=200x^100; P`(1)=20000
Med(T(4,4)S[5,15]): CJS(x)=600x^75; P`(1)=45000; $PI_v$(x)=300x^150; P`(1)=45000
Med(T(4,4)S[5,20]): CJS(x)=800x^100; P`(1)=80000; $PI_v$(x)=400x^200; P`(1)=80000
Med(T(4,4)S[5,10]): CJP(x)=200x^2500; P`(1)=500000; *v*=100; *e*= 200.
Med(T(4,4)S[5,15]): CJP(x)=300x^5625; P`(1)= 1687500; *v*=150; *e*= 300.
Med(T(4,4)S[5,20]): CJP(x)=400x^10000; P`(1)= 4000000; *v*=200; *e*= 400.

For an edge $e \in E(G)$, let $c(e) := \{f \in E(G); f\ co\ e\}$ be the set of edges codistant to *e* in *G*. The set *c*(*e*) can be obtained by an *orthogonal cut oc* of *G*, with respect to *e*. If *G* is a *co-graph* then its orthogonal cuts form a partition in *G* (see above). A bipartite graph *G* is a *co-graph* if and only if it is a *partial cube*, and all its semicubes are convex. However, a *co*-graph can also be non-bipartite [32] (*e.g.*, it shows a transitive *co*-relation but has at least one odd cycle, thus being no more a partial cube). It was proven that relation *co* is a *theta* (Djoković [50]) and Winkler [51]) relation.

Two edges *e* and *f* of a plane graph *G* are in relation *opposite, e op f,* if they are opposite edges of an inner face of *G*. Then *e co f* holds by assuming the faces are isometric. Note that relation *co* involves distances in the whole graph while *op* is defined only locally (it relates face-opposite edges). If *G* is a *co*-graph, then its opposite edge strips *ops* $\{s_k\}$ superimpose over the orthogonal cut sets *ocs* $\{c_k\}$ and $|c_k|=|s_k|$.

Using the relation *op* we can partition the edge set of *G* into *opposite* edge *strips, ops*: any two subsequent edges of an *ops* are in *op* relation and any three subsequent edges of such a strip belong to adjacent faces. Note that John *et al*. [49] implicitly used the "*op*" relation in defining the Cluj-Ilmenau index *CI* (see below).

Let us denote by *m*(*s*) or simply *m* the number of *ops* of length $s=|s_k|$ and define the Omega polynomial as [52-55]:

$$\Omega(x) = \sum_s m \cdot x^s \qquad (13)$$

The exponents count just the intersected edges by the cut-line (in a cutting procedure), which does not need to be orthogonal on all the edges of an *ops.*

In *co*-graphs/partial cubes, other two related polynomials [48] can be calculated:

$$\Theta(x) = \sum_s ms \cdot x^s \qquad (14)$$

$$\Pi(x) = \sum_s ms \cdot x^{e-s} \qquad (15)$$

The above polynomials count codistant and non-codistant edges, respectively. Thus, non-co-distance is related to edge-proximity, and the name of these polynomials is immediate.

The first derivative (computed at x=1) of these counting polynomials provide interesting topological indices [48]:

$$\Omega'(1) = \sum_s ms = e = |E(G)| \qquad (16)$$

$$\Theta'(1) = \sum_s ms^2 = \Theta(G) \qquad (17)$$

$$\Pi'(1) = \sum_s ms(e-s) = \Pi(G) \qquad (18)$$

On $\Omega(x)$ an index, called Cluj-Ilmenau [49] *CI*(*G*), was defined

$$CI(G) = \left\{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\right\} \qquad (19)$$

In *co*-graphs, there is the equality [48]: $CI(G) = \Pi(G)$. This result can be obtained applying the definition (19):

$$CI(G) = \left(\sum_s ms\right)^2 - \left[\sum_s ms + \sum_s ms(s-1)\right] = e^2 - \sum_s ms^2 = \Pi(G) \qquad (20)$$

Relation (20) is just the formula proposed by John *et al*. [56] to calculate the Khadikar's *PI* index [34]. According to Ashrafi's notations [57], PI_e (to difer from PI_v) can be written as:

$$PI_e(G) = \sum_{e \in E(G)} \left[n(e,u) + n(e,v)\right] - m(u,v) \qquad (21)$$

where *n*(*e*,*u*) is the number of edges lying closer to the vertex *u* than to the *v* vertex while *m*(*u*,*v*) is the number of edges equidistant from *u* and *v*.

This index can be calculated as the first derivative, in x=1, of the polynomial defined by Ashrafi [57] as:

$$PI_e(x) = \sum_{e \in E(G)} x^{n(e,u)+n(e,v)} \qquad (22)$$

In bipartite graphs, either *co*-graphs or not, the equality: $\Pi(G) = PI_e(G)$ is true, but not in general graphs. In partial cubes, since they are also bipartite, the previous equality can be expanded to

$$CI(G) = \Pi(G) = PI_e(G) \tag{23}$$

a relation precisely true in partial cubes but not in all *co*-graphs (e.g., in non-bipartite co-graphs). As the rhomb-tiled tori are not *co*-graphs, then $CI(G) \neq \Pi(G)$.

Formulas for the above three polynomials in rhomb-tiled tori T(4,4)R[*c*,*n*] are given in Table 2, along with some examples.

Table 2. Polynomials of Edge Proximity in tori T(4,4)R[*c*,*n*] designed by Med(T(4,4)S[*c*,*n*]); vertex multiplicity *m*=2.

Formulas	
$\Omega(x) = 2c \cdot x^{2n}$	$\Pi(x) = e \cdot x^{e-(6c-2)}$
$CI = 16c^2n^2 - 8cn^2$	$\Pi'(1) = e[e-(6c-2)]$
$\Theta(x) = 2c \cdot 2n \cdot x^{6c-2} = e \cdot x^{6c-2}$	$v = cn$; $e = 2c \cdot 2n$
$\Theta'(1) = e \cdot (6c-2)$	

Examples	
T[**10**,30]; $\Omega(x)$ =20x^{60}; CI=1368000;	$\Theta(x)$ =1200x^{58}; $\Theta'(1)$ = 69600;
	$\Pi(x)$ =1200x^{1142}; $\Pi'(1)$ =1370400
T[**15**,30]; $\Omega(x)$ =30x^{60}; CI=3132000;	$\Theta(x)$ =1800x^{88}; $\Theta'(1)$ =158400;
	$\Pi(x)$ =1800x^{1712}; $\Pi'(1)$ =3081600
T[**10**,40]; $\Omega(x)$ =20x^{80}; CI=2432000;	$\Theta(x)$ =1600x^{58}; $\Theta'(1)$ =92800;
	$\Pi(x)$ =1600x^{1542}; $\Pi'(1)$ =2467200

CONCLUSIONS

Cluj and Omega polynomials can be defined on the ground of an orthogonal cutting procedure. Some other related counting polynomials were derived by the cutting procedure. Formulas to calculate these polynomials in T(4,4)R[*c*,*n*] tori were given and exemplified.

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